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Title :, On the Role of Stone-Wales Defects on the Performance of Graphene Nanoribbon Photo Detectors

Authors: Mahdi Moradinasab

Abstract

The electronic and optical properties Graphene nanoribbons depend on the chirality of the edges and on the width. The edges of nanoribbons can be of zigzag or armchair type, or a combination of these two. Zigzag nanoribbons show metallic properties, whereas armchair ribbons are semiconductors. It has been theoretically predicted that zizgag edges can rearrange to produce Stone-Wales defects [1]. Recently, the presence of this kind of edge reconstruction has been observed experimentally [2]. As the electrical and optical properties of nanoribbons strongly depend on the edge type, such structures can have properties very different from that of perfect zigzag ribbons. The electronic properties of these structures have studied in Refs. [3-4]. In the present work we investigate the optical properties of these structures using first-principles calculation and analyse their performance as infra-red photo-detectors. First-principles calculations were carried out using the ab initio pseudopotential spin density functional theory to obtain the relaxed atomic positions and the electronic structure. Dielectric function, optical conductivity, and quantum efficiency of photo-detectors based on these materials are investigated. Our results indicate that in edge-reconstructed structures, photon absorption occurs in a wider spectrum than in structures without edge reconstruction. Furthermore, the absorption peaks shift to larger wave lengths in the edge-reconstructed structures. In this way, quantum efficiency for infra-red photo-detection is improved. The presented study shows that edge-reconstructed zigzag nanoribbons are potential candidates for future infra-red optoelectronic applications.

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